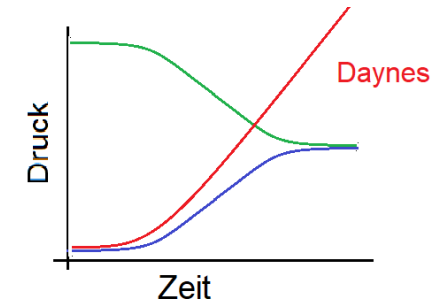
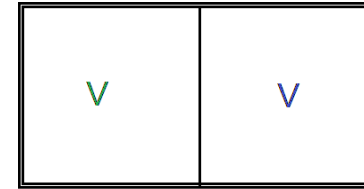
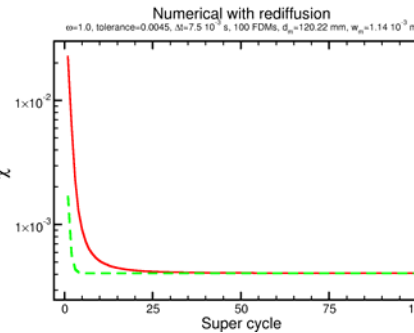
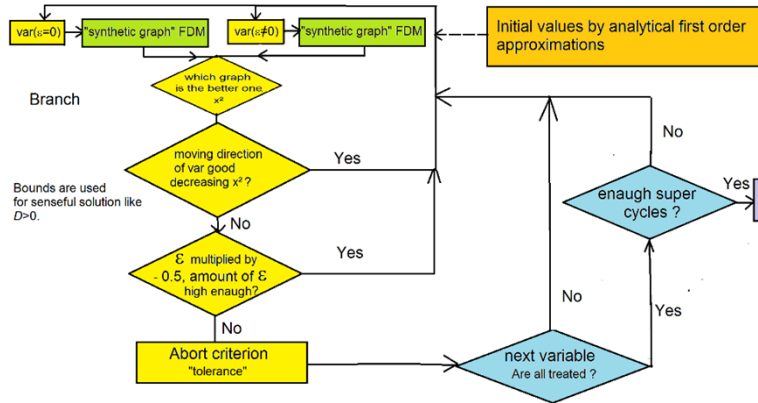


Neue Lösungen der Kontinuitätsdifferentialgleichung mit Phasengleichgewicht zur Verbesserung der Ergebnisse bei der Auswertung von Experimenten, MathSEE

A. von der Weth¹, F. Arbeiter¹, R. Dagan², D. Klimenko¹, K. Nagatou³, V. Pasler¹, G. Schlindwein¹, M. Schulz³, K. Zinn¹. 1: INR 2: INE 3: IANA, Karlsruhe 11. 12. 2019

Bestimmung von Transportparametern aus gemessener Kurve mittels B&B branch and bound Algorithmus

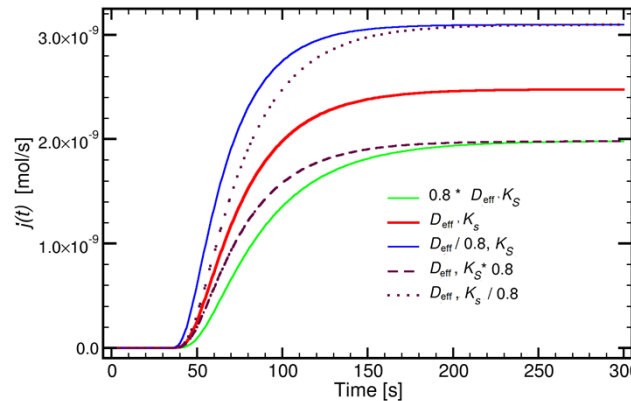


$$j(t)_{measure} = \frac{D_{eff} c(0) d_m^2}{w_m 4 \pi} \left(1 + 2 \sum_{k=1}^{\infty} (-1)^k e^{-\frac{k^2 \pi^2 D_{eff} (t-t_{off})}{w_m^2}} \right)$$

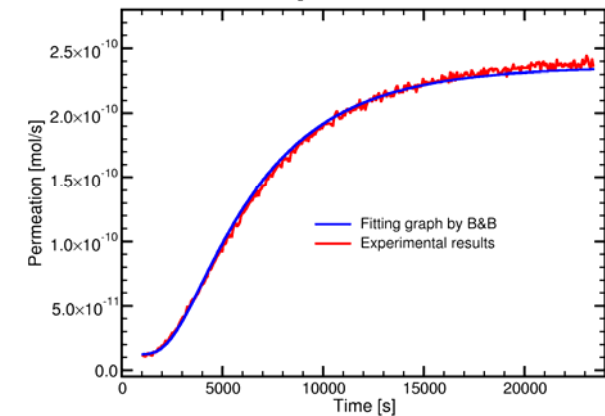
Daynes Lösung bekannt, aber nicht anwendbar!

super cycle	bounds
1. $t_{off}; t_{off} + \epsilon$	
2. $D_{eff}; D_{eff} (1 + \epsilon)$	$D_{eff} > 0$
3. $c(0); c(0)(1 + \epsilon)$	$c(0) > 0$
4. $D_{eff}, c(0); D_{eff} (1 + \epsilon), c(0)/(1 + \epsilon)$	$j_{steady state} = const.$
5. $j_{offset}; j_{offset} (1 + \epsilon)$	$j_{offset} > 0$

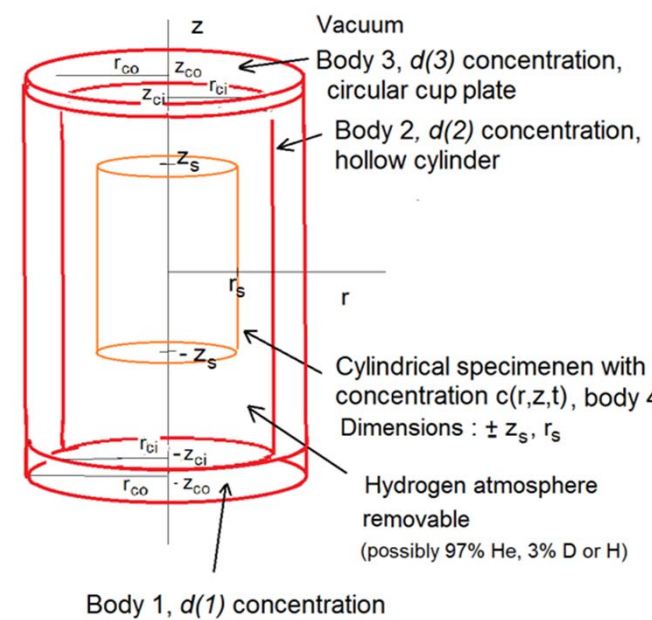
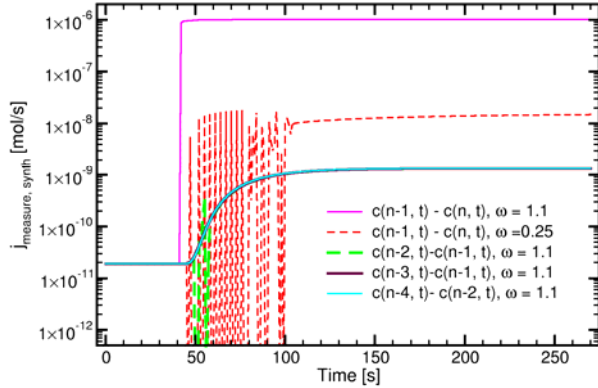
$T = 573 \text{ K}, D_{st} = 4.78 \cdot 10^{-9} \text{ m}^2/\text{s}, K_{s,st} = 5.06 \cdot 10^{-2} \text{ mol}/\text{m}^3$
 $p_L = 3 \cdot 10^3 \text{ Pa}, \dot{m} = 180 \text{ ml}/\text{min}, d_m = 1.2 \text{ mm}, w_m = 125 \text{ mm}$



Numerical with rediffusion, $D = 3.07 \cdot 10^{-11} \text{ m}^2/\text{s}, k_{s,sa} = 0.036 \text{ mol}/\text{m}^3/\text{Pa}^{0.5}$
 $p_L = 420 \text{ Pa}, 300 \text{ sccm}$



T=673 K, Optifer, 150 Pa, $w_m = 125$ mm, $d_m = 1.2$ mm, 30 ml/min
 ω SOR parameter, $n=100$



$$\vec{c}_{k+1} = \vec{c}_k + D^* \begin{pmatrix} 0 \\ D^* - 2D^* D^* \\ D^* - 2D^* D^* \\ D^* - 2D^* D^* \\ \vdots \\ D^* - 2D^* D^* \\ 0 \end{pmatrix} \vec{c}_{k+1} = \begin{pmatrix} 1 \\ -D^* 1+2D^* -D^* \\ -D^* 1+2D^* -D^* \\ -D^* 1+2D^* -D^* \\ \vdots \\ -D^* 1+2D^* -D^* \\ -D^* 1+2D^* -D^* \\ 1 \end{pmatrix} \vec{c}_k$$

$$D^* = \frac{D \Delta t}{\Delta X^2}$$

$$\frac{\partial c}{\partial t} = D_{sa} \Delta c$$

$$\frac{\partial d(i)}{\partial t} = D_{cu} \Delta d(i), i = 1,2,3$$

Randbedingungen in Auswahl:

$$c(0 \leq r \leq r_s, z = \pm z_s, \forall t) = k_{s,sa} \sqrt{p(t)}$$

$$c(r = r_s, |z| \leq z_s, \forall t) = k_{s,sa} \sqrt{p(t)}$$

$$d(1)(r \leq r_{co}, z = -z_{ci}, \forall t) = k_{s,cu} \sqrt{p(t)}$$

$$\frac{dm}{dt} = -2 \pi D_{sa} \int_0^{r_s} \underbrace{2}_{symmetric} r \frac{\partial}{\partial z} c(r, z = z_s, t) dr - \underbrace{2 \pi r_s D_{sa} \int_{-z_s}^{z_s} \frac{\partial}{\partial r} c(r = r_s, z, t) dz}_{superficies surface of specimen}$$

$$2 \pi D_{cu} \int_0^{r_{co}} r \frac{\partial}{\partial z} d(1)(r, z = -z_{ci}, t) dr - 2 \pi r_{ci} D_{cu} \int_{-z_{ci}}^{z_{ci}} \frac{\partial}{\partial r} d(2)(r = r_{ci}, z, t) dz -$$

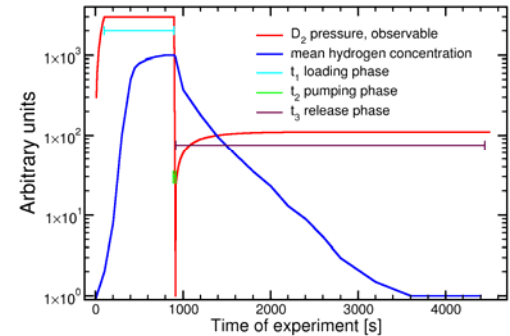
circular aerea of body 1 superficies surface of body 2

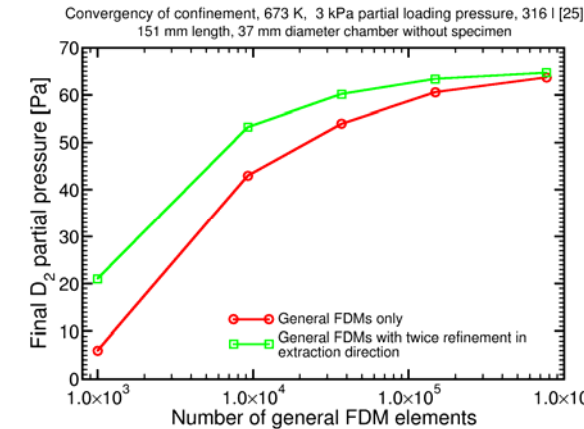
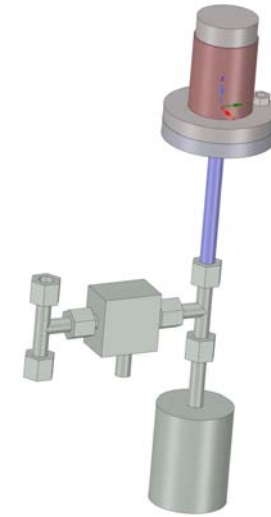
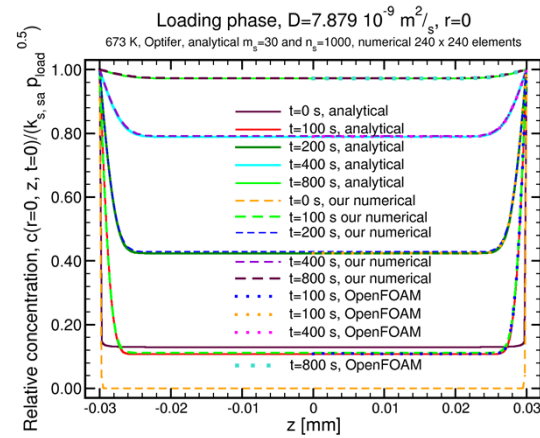
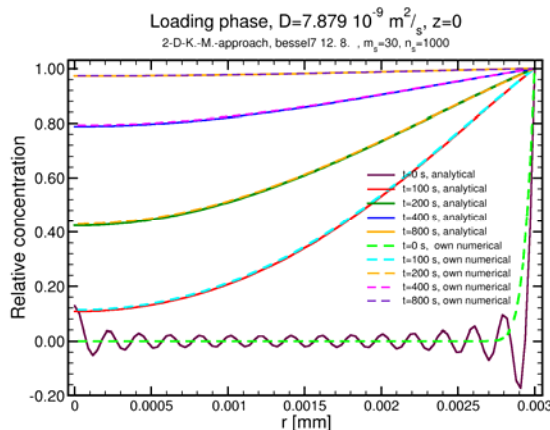
$$2 \pi D_{cu} \int_0^{r_{co}} r \frac{\partial}{\partial z} d(3)(r, z = z_{ci}, t) dr$$

circular area of body 3

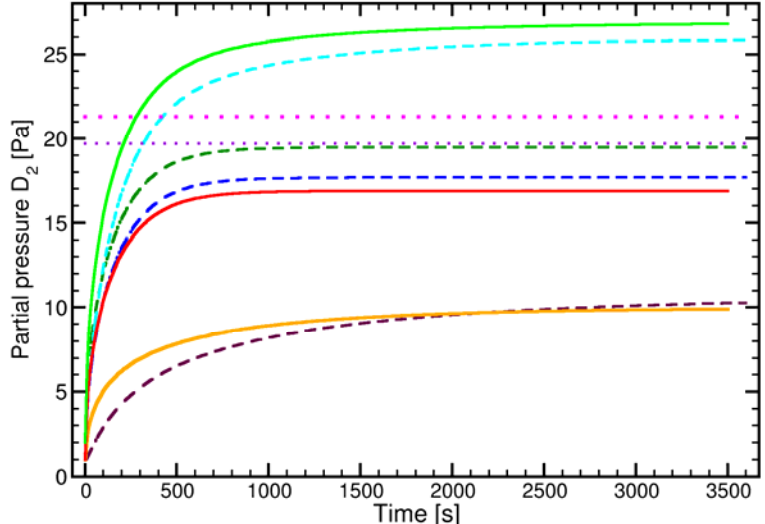
$$p(t) = p_{start} + \underbrace{\frac{k_v}{RT_{abs}}}_{RT_{abs}/V_{gas}} \int_{t_1+t_2}^t \underbrace{0.5}_{gaseous \leftrightarrow interstitial} \frac{dm}{dt} dt$$

Principle sketch of GR experimental flow





Optifer, 673K, $p_{\text{load}} = 3 \text{ kPa}$, $r_{\text{ci}} = 10 \text{ mm}$, $r_{\text{co}} = 20 \text{ mm}$, $z_{\text{ci}} = 40 \text{ mm}$, $z_{\text{co}} = 50 \text{ mm}$
 $D_{\text{sa}} = 7.879 \cdot 10^{-9} \text{ m}^2/\text{s}$, $k_{\text{s,sa}} = 1.829 \cdot 10^{-3} \text{ mol/m}^2/\text{Pa}^{0.5}$, $r_{\text{sa}} = 3 \text{ mm}$, $z_{\text{sa}} = 30 \text{ mm}$, $D_{\text{cu}} = 8.257 \cdot 10^{-10} \text{ m}^2/\text{s}$, $k_{\text{s,cu}} = 5.914 \cdot 10^{-4} \text{ mol/m}^2/\text{Pa}^{0.5}$



- Confinement only, 27600 FDM elements
- Specimen only, $9 \cdot 10^4$ FDM elements
- "Analytical" solution with $4.9 \cdot 10^5$ FDM elements
- Specimen with interacting confinement
- Case of total hydrogen evaporation from specimen
- Case of "analytical" solution with phase equilibrium
- Analytical solution of confinement
- Analytical solution of specimen
- Analytical solution confinement and specimen

Acknowledgement:

The current talk summarizes results of two running projects:

Main goal of the first one is the determination of transport parameters of hydrogen in structural metallic materials used for components in fusion power stations:
This work has been carried out within the framework of the EUROfusion Consortium, and has received funding from the Euratom research and training program 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission

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Neue Lösungen der Kontinuitätsdifferentialgleichung mit Phasengleichgewicht zur Verbesserung der Ergebnisse bei der Auswertung von Experimenten.

